

Data Path : Z:\voasrv\HPCHEM1\MSVOA_U\Data\VU062024\
 Data File : VU059372.D
 Acq On : 20 Jun 2024 12:10
 Operator : MD/SY
 Sample : P2897-07ME
 Misc : 4.89g/5.0mL/100uL/5.0mL/MSVOA_U/MEOH
 ALS Vial : 9 Sample Multiplier: 1

Instrument :
 MSVOA_U
 ClientSampleId :
 C0SB7ME

Integration Parameters: LSCINT.P

Integrator: RTE

Smoothing : OFF

Filtering: 5

Sampling : 1

Min Area: 0 % of largest Peak

Start Thrs: 0.2

Max Peaks: 100

Stop Thrs : 0

Peak Location: TOP

If leading or trailing edge < 100 prefer < Baseline drop else tangent >

Peak separation: 5

Method : Z:\voasrv\HPCHEM1\MSVOA_U\Method\SFAMULM052924WMA.M
 Title : VOC Analysis

Signal : TIC: VU059372.D\data.ms

peak #	R.T. min	first scan	max scan	last scan	PK TY	peak height	corr. area	corr. % max.	% of total
1	1.480	54	59	65	rBV4	1999	2201	0.32%	0.034%
2	1.592	87	94	117	rVB	36254	61737	9.03%	0.947%
3	1.824	134	166	167	rBV4	44266	161345	23.60%	2.475%
4	2.473	365	368	371	rBV2	410	319	0.05%	0.005%
5	2.537	376	388	404	rVB	95948	155793	22.79%	2.390%
6	2.618	408	413	414	rBV	462	357	0.05%	0.005%
7	2.763	451	458	464	rBV3	720	1111	0.16%	0.017%
8	2.946	504	515	529	rBV	12719	26821	3.92%	0.411%
9	3.029	532	541	556	rVB3	3423	6728	0.98%	0.103%
10	3.168	577	584	591	rVV3	966	1550	0.23%	0.024%
11	3.197	591	593	599	rVB3	589	535	0.08%	0.008%
12	3.293	617	623	626	rBV2	283	421	0.06%	0.006%
13	3.653	731	735	737	rBV	326	284	0.04%	0.004%
14	3.824	784	788	791	rBV2	190	208	0.03%	0.003%
15	3.946	821	826	830	rBV	218	219	0.03%	0.003%
16	4.094	869	872	878	rVB2	204	244	0.04%	0.004%
17	4.174	891	897	902	rVB2	354	463	0.07%	0.007%
18	4.312	935	940	945	rBV	288	387	0.06%	0.006%
19	4.624	1026	1037	1082	rBV	42922	136151	19.92%	2.089%
20	4.888	1114	1119	1123	rBV3	332	356	0.05%	0.005%
21	4.949	1135	1138	1141	rVB3	347	275	0.04%	0.004%
22	4.968	1141	1144	1149	rVB	425	325	0.05%	0.005%
23	5.052	1153	1170	1195	rBV	92185	211334	30.91%	3.242%
24	5.142	1195	1198	1202	rVV2	417	404	0.06%	0.006%
25	5.168	1202	1206	1210	rVV3	285	304	0.04%	0.005%
26	5.219	1219	1222	1226	rVB2	264	233	0.03%	0.004%
27	5.325	1250	1255	1261	rVB2	258	229	0.03%	0.004%
28	5.486	1301	1305	1307	rBV	251	209	0.03%	0.003%
29	5.553	1323	1326	1331	rBV2	342	330	0.05%	0.005%
30	5.589	1334	1337	1341	rBV2	294	269	0.04%	0.004%
31	5.711	1356	1375	1403	rBV2	199333	525924	76.93%	8.069%
32	5.901	1429	1434	1436	rVV2	207	210	0.03%	0.003%
33	5.968	1450	1455	1456	rBV2	645	528	0.08%	0.008%
34	6.238	1525	1539	1567	rBV	265363	523275	76.55%	8.028%
35	6.521	1620	1627	1638	rVB8	2953	5874	0.86%	0.090%
36	6.595	1638	1650	1653	rBV4	1433	1865	0.27%	0.029%

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 ClientSampleId :
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Integration Parameters: LSCINT.P

Integrator: RTE

Smoothing : OFF

Filtering: 5

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Method : Z:\voasrv\HPCHEM1\MSVOA_U\Method\SFAMULM052924WMA.M
 Title : VOC Analysis

37	6.682	1664	1677	1697	rBV	118450	233878	34.21%	3.588%
38	6.753	1697	1699	1703	rVB2	684	341	0.05%	0.005%
39	6.875	1734	1737	1742	rVB2	288	262	0.04%	0.004%
40	6.965	1761	1765	1770	rBV2	352	385	0.06%	0.006%
41	7.055	1789	1793	1796	rBV	279	279	0.04%	0.004%
42	7.200	1830	1838	1844	rVV5	1749	2850	0.42%	0.044%
43	7.225	1844	1846	1853	rVB4	783	695	0.10%	0.011%
44	7.261	1853	1857	1863	rVB	383	392	0.06%	0.006%
45	7.373	1889	1892	1897	rVB2	249	262	0.04%	0.004%
46	7.489	1925	1928	1932	rVB	333	214	0.03%	0.003%
47	7.560	1936	1950	1969	rBV	57759	106616	15.60%	1.636%
48	7.695	1986	1992	1993	rBV2	541	408	0.06%	0.006%
49	7.891	2041	2053	2075	rBV	222609	393106	57.50%	6.031%
50	8.042	2096	2100	2103	rBV2	365	276	0.04%	0.004%
51	8.177	2132	2142	2158	rVV2	39241	71978	10.53%	1.104%
52	8.238	2158	2161	2165	rVB	334	291	0.04%	0.004%
53	8.299	2172	2180	2183	rBV2	210	307	0.04%	0.005%
54	8.412	2211	2215	2221	rBV2	368	445	0.07%	0.007%
55	8.547	2247	2257	2268	rVB4	3833	5625	0.82%	0.086%
56	8.640	2274	2286	2321	rBV2	117319	286199	41.87%	4.391%
57	8.917	2365	2372	2378	rVB	220	338	0.05%	0.005%
58	9.142	2436	2442	2444	rBV	237	282	0.04%	0.004%
59	9.212	2458	2464	2466	rBV2	342	295	0.04%	0.005%
60	9.412	2513	2526	2554	rBV	381194	681207	99.65%	10.451%
61	9.614	2585	2589	2595	rBV2	286	301	0.04%	0.005%
62	9.698	2610	2615	2622	rBV2	1261	1457	0.21%	0.022%
63	9.746	2625	2630	2633	rVB3	565	396	0.06%	0.006%
64	9.807	2646	2649	2654	rVB2	331	277	0.04%	0.004%
65	9.904	2674	2679	2686	rVB2	363	461	0.07%	0.007%
66	10.084	2732	2735	2740	rVV2	328	312	0.05%	0.005%
67	10.183	2762	2766	2769	rBV2	245	213	0.03%	0.003%
68	10.248	2780	2786	2793	rBV4	686	763	0.11%	0.012%
69	10.319	2802	2808	2811	rBV2	233	226	0.03%	0.003%
70	10.389	2825	2830	2836	rBV3	835	946	0.14%	0.015%
71	10.598	2890	2895	2897	rBV2	455	330	0.05%	0.005%
72	10.618	2897	2901	2902	rVV2	645	486	0.07%	0.007%
73	10.634	2904	2906	2908	rVV2	902	552	0.08%	0.008%
74	10.650	2908	2911	2916	rVV5	1119	1093	0.16%	0.017%
75	10.753	2931	2943	2957	rBV	193223	327247	47.87%	5.021%
76	11.007	3019	3022	3028	rVB2	603	480	0.07%	0.007%

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Instrument :
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 ClientSampleId :
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Integration Parameters: LSCINT.P

Integrator: RTE

Smoothing : OFF

Filtering: 5

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Peak Location: TOP

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Method : Z:\voasrv\HPCHEM1\MSVOA_U\Method\SFAMULM052924WMA.M
 Title : VOC Analysis

77	11.061	3028	3039	3046	rBV6	1452	2383	0.35%	0.037%
78	11.113	3047	3055	3068	rVV5	7690	12641	1.85%	0.194%
79	11.193	3079	3080	3085	rVB3	479	315	0.05%	0.005%
80	11.261	3098	3101	3105	rBV	414	427	0.06%	0.007%
81	11.283	3105	3108	3111	rVV4	623	434	0.06%	0.007%
82	11.302	3111	3114	3125	rVB8	1627	2742	0.40%	0.042%
83	11.351	3125	3129	3130	rBV2	618	428	0.06%	0.007%
84	11.367	3132	3134	3135	rBV2	531	219	0.03%	0.003%
85	11.412	3140	3148	3156	rBV6	6025	8896	1.30%	0.136%
86	11.569	3194	3197	3201	rVB3	817	608	0.09%	0.009%
87	11.640	3213	3219	3224	rVB5	2650	2781	0.41%	0.043%
88	11.708	3231	3240	3246	rBV8	3090	5101	0.75%	0.078%
89	11.810	3260	3272	3287	rBV	414483	683617	100.00%	10.488%
90	12.190	3378	3390	3406	rBV	249404	421427	61.65%	6.465%
91	12.322	3424	3431	3443	rVB	29118	41970	6.14%	0.644%
92	12.662	3530	3537	3546	rBV5	6921	9723	1.42%	0.149%
93	13.045	3651	3656	3665	rVB6	18114	25092	3.67%	0.385%
94	13.425	3767	3774	3794	rVB2	64630	125133	18.30%	1.920%
95	13.582	3817	3823	3829	rBV3	25303	37856	5.54%	0.581%
96	14.444	4084	4091	4100	rBV	124376	166665	24.38%	2.557%
97	15.203	4322	4327	4339	rVB2	71782	100132	14.65%	1.536%
98	15.395	4380	4387	4396	rVB	203865	267330	39.11%	4.101%
99	15.971	4561	4566	4579	rVB	141579	193100	28.25%	2.962%
100	16.286	4657	4664	4675	rVB	335434	457849	66.97%	7.024%

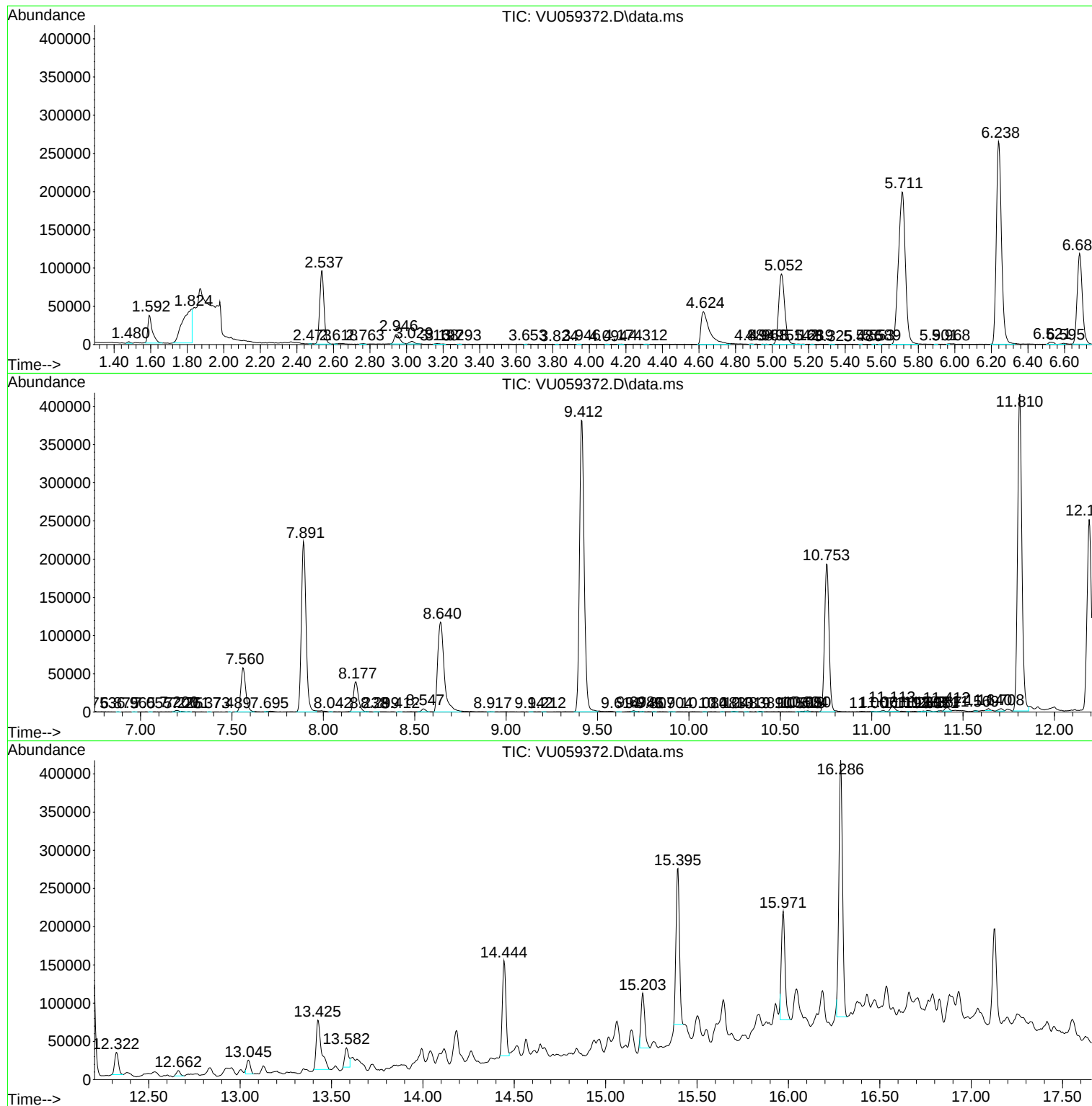
Sum of corrected areas: 6518158

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ALS Vial : 9 Sample Multiplier: 1

Instrument :
MSVOA_U
ClientSampleId :
C0SB7ME

Quant Method : Z:\voasrv\HPCHEM1\MSVOA_U\Method\SFAMULM052924WMA.M
Quant Title : VOC Analysis

TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P



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ALS Vial : 9 Sample Multiplier: 1

Instrument :
MSVOA_U
ClientSampleId :
C0SB7ME

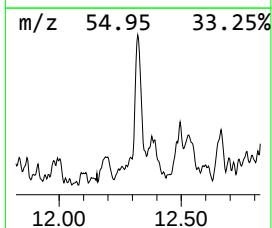
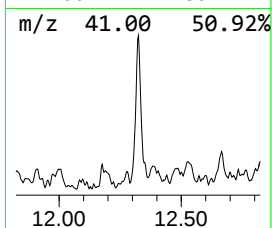
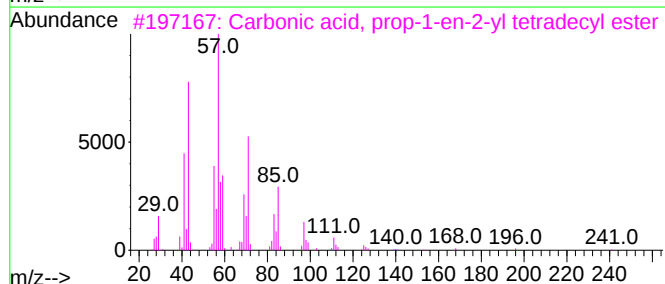
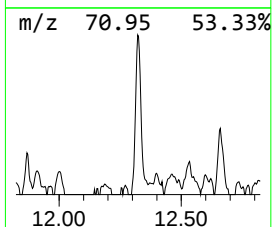
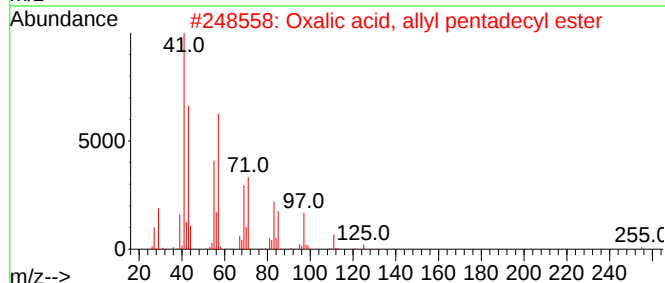
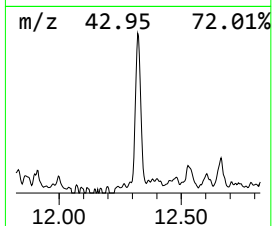
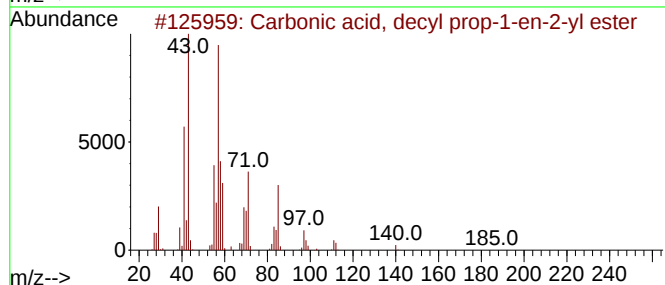
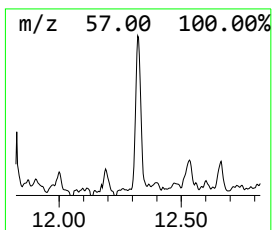
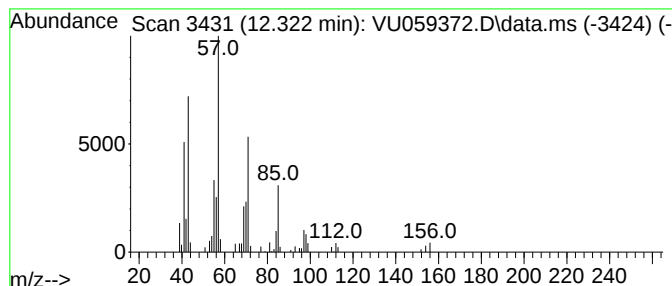
Quant Method : Z:\voasrv\HPCHEM1\MSVOA_U\Method\SFAMULM052924WMA.M
Quant Title : VOC Analysis

TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

Peak Number 2 Carbonic acid, decyl prop-1... Concentration Rank 8

R.T.	EstConc	Area	Relative to ISTD	R.T.
12.322	3.07 ug/L	41970	1,4-Dichlorobenzene-d4	11.810

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Carbonic acid, decyl prop-1-en-2...	242	C14H26O3	1000382-90-5	90
2			Oxalic acid, allyl pentadecyl ester	340	C20H36O4	1000309-24-3	86
3			Carbonic acid, prop-1-en-2-yl te...	298	C18H34O3	1000382-90-9	72
4			Carbonic acid, nonyl prop-1-en-2...	228	C13H24O3	1000382-53-9	64
5			Carbonic acid, octyl prop-1-en-2...	214	C12H22O3	1000382-54-0	64



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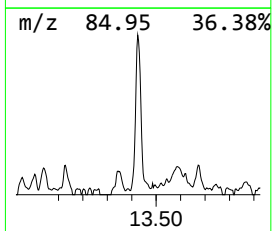
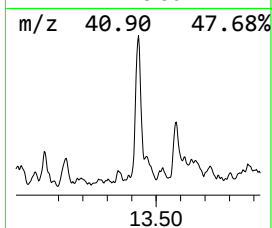
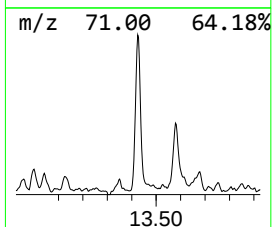
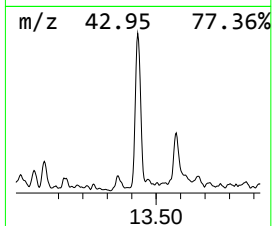
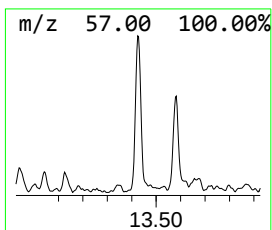
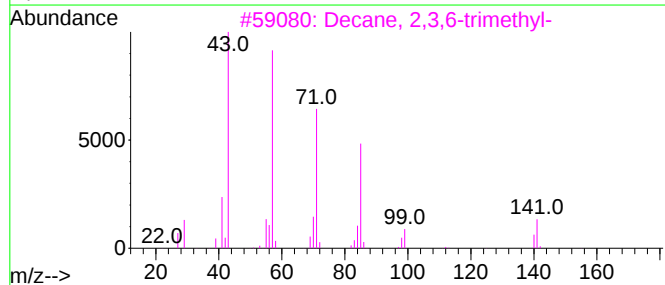
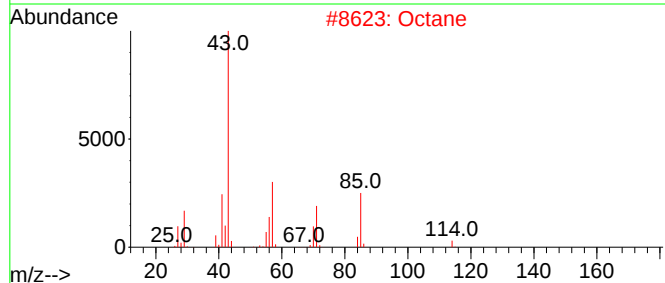
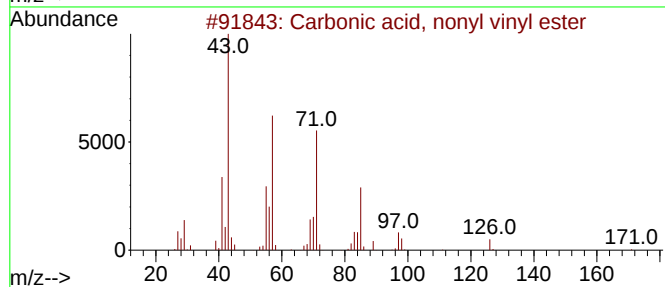
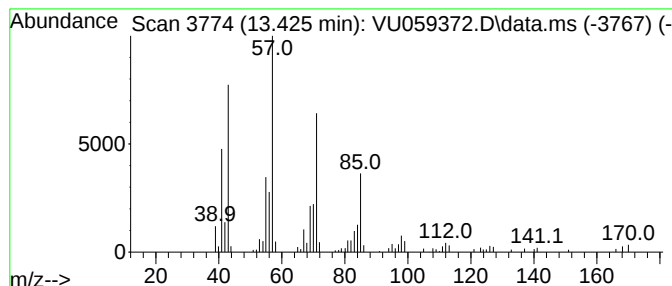
Quant Method : Z:\voasrv\HPCHEM1\MSVOA_U\Method\SFAMULM052924WMA.M
Quant Title : VOC Analysis

TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

Peak Number 3 Carbonic acid, nonyl vinyl ... Concentration Rank 6

R.T.	EstConc	Area	Relative to ISTD	R.T.
13.425	9.15 ug/L	125133	1,4-Dichlorobenzene-d4	11.810

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Carbonic acid, nonyl vinyl ester	214	C12H22O3	1000383-25-6	86
2			Octane	114	C8H18	000111-65-9	64
3			Decane, 2,3,6-trimethyl-	184	C13H28	062238-12-4	59
4			2,6-Dimethyldecane	170	C12H26	013150-81-7	58
5			Decane, 2,4-dimethyl-	170	C12H26	002801-84-5	50



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ALS Vial : 9 Sample Multiplier: 1

Instrument :
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ClientSampleId :
C0SB7ME

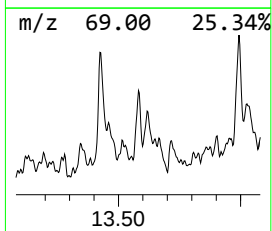
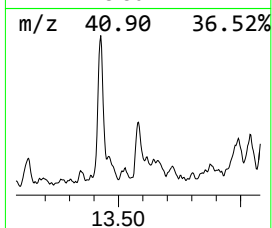
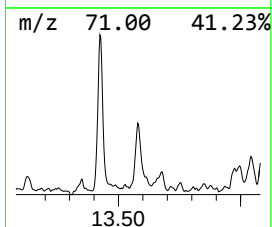
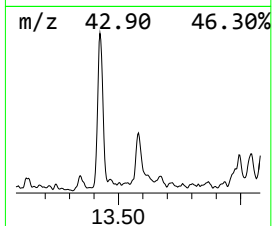
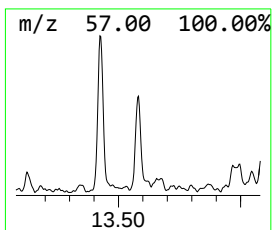
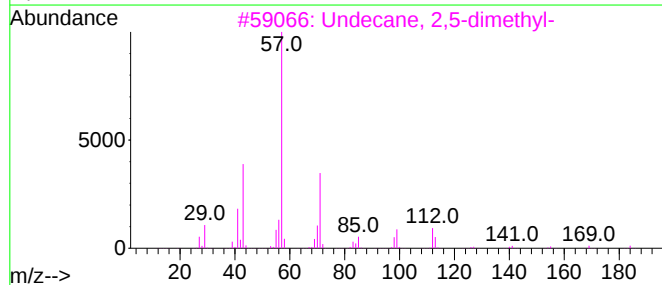
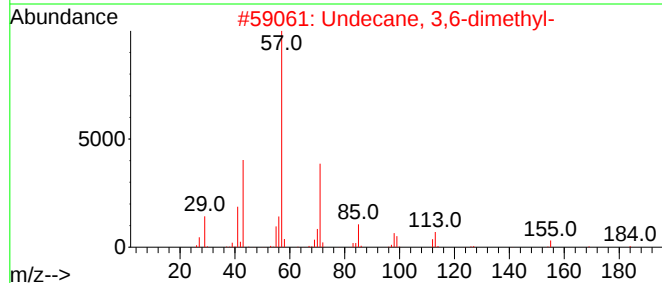
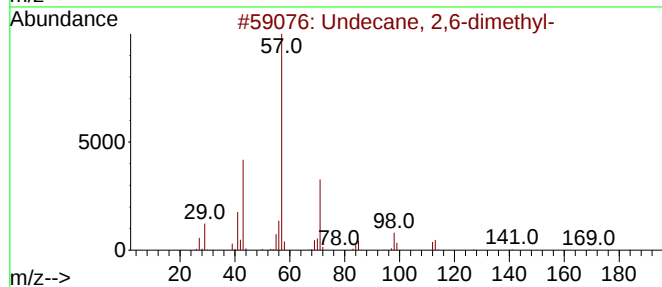
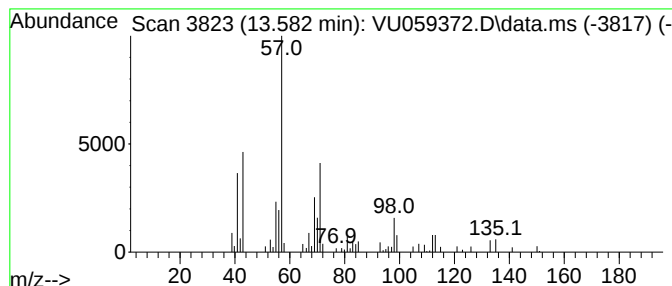
Quant Method : Z:\voasrv\HPCHEM1\MSVOA_U\Method\SFAMULM052924WMA.M
Quant Title : VOC Analysis

TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

Peak Number 4 (DEL) Alkane: Straight-Chai... Concentration Rank 9

R.T.	EstConc	Area	Relative to ISTD	R.T.
13.582	2.77 ug/L	37856	1,4-Dichlorobenzene-d4	11.810

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Undecane, 2,6-dimethyl-	184	C13H28	017301-23-4	72
2			Undecane, 3,6-dimethyl-	184	C13H28	017301-28-9	64
3			Undecane, 2,5-dimethyl-	184	C13H28	017301-22-3	53
4			Octane, 3,6-dimethyl-	142	C10H22	015869-94-0	53
5			Nonane, 3-methyl-	142	C10H22	005911-04-6	53



Data Path : Z:\voasrv\HPCHEM1\MSVOA_U\Data\VU062024\
Data File : VU059372.D
Acq On : 20 Jun 2024 12:10
Operator : MD/SY
Sample : P2897-07ME
Misc : 4.89g/5.0mL/100uL/5.0mL/MSVOA_U/MEOH
ALS Vial : 9 Sample Multiplier: 1

Instrument :
MSVOA_U
ClientSampleId :
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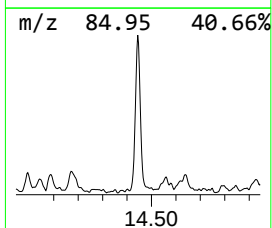
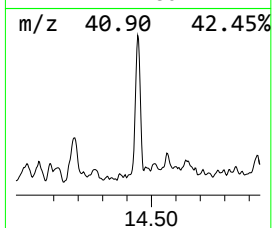
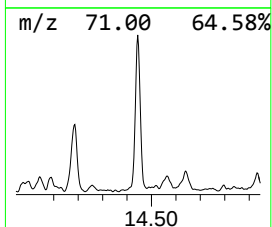
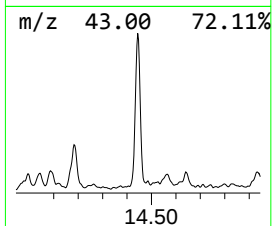
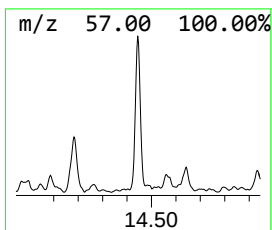
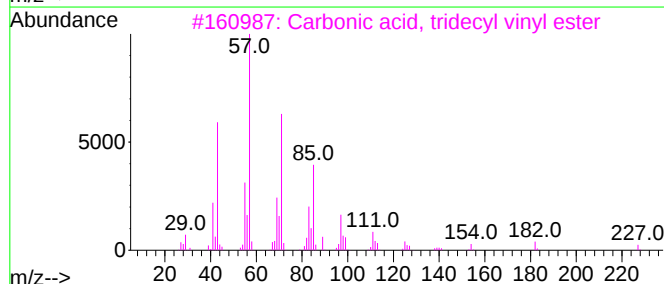
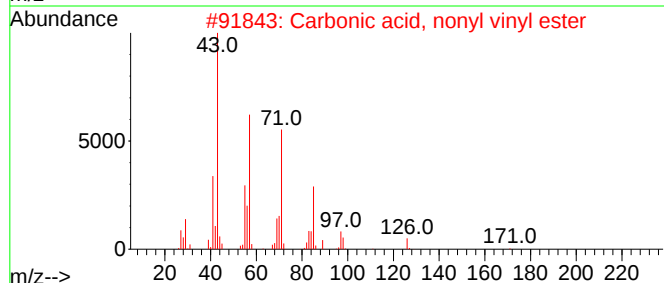
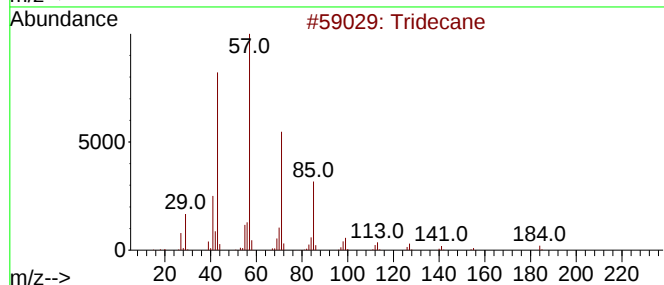
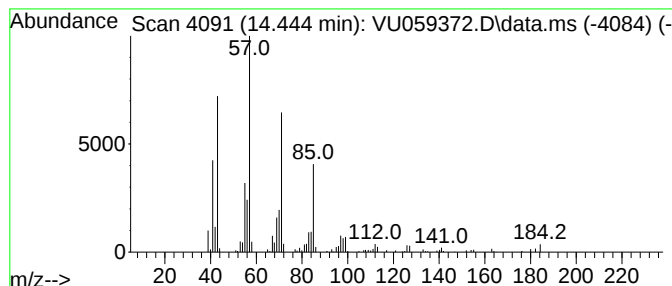
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Quant Title : VOC Analysis

TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

Peak Number 5 (DEL) Alkane: Straight-Chai... Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.
14.444	12.19 ug/L	166665	1,4-Dichlorobenzene-d4	11.810

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Tridecane	184	C13H28	000629-50-5	87
2			Carbonic acid, nonyl vinyl ester	214	C12H22O3	1000383-25-6	80
3			Carbonic acid, tridecyl vinyl ester	270	C16H30O3	1000382-54-7	78
4			Nonadecane	268	C19H40	000629-92-5	72
5			Tridecane	184	C13H28	000629-50-5	64



Data Path : Z:\voasrv\HPCHEM1\MSVOA_U\Data\VU062024\
Data File : VU059372.D
Acq On : 20 Jun 2024 12:10
Operator : MD/SY
Sample : P2897-07ME
Misc : 4.89g/5.0mL/100uL/5.0mL/MSVOA_U/MEOH
ALS Vial : 9 Sample Multiplier: 1

Instrument :
MSVOA_U
ClientSampleId :
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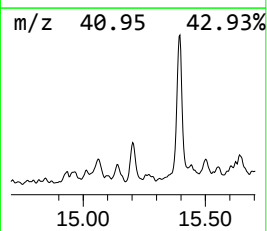
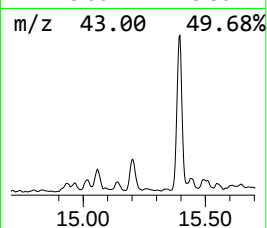
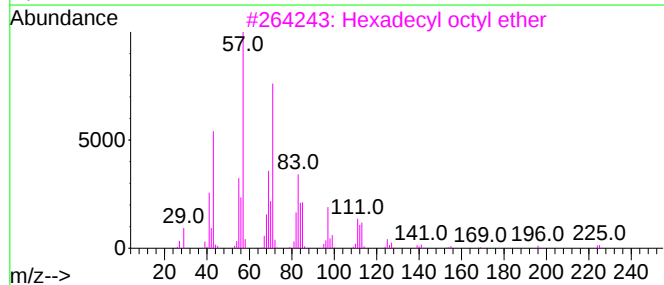
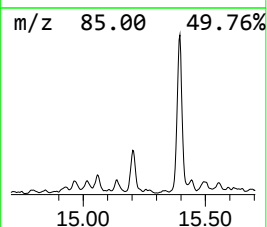
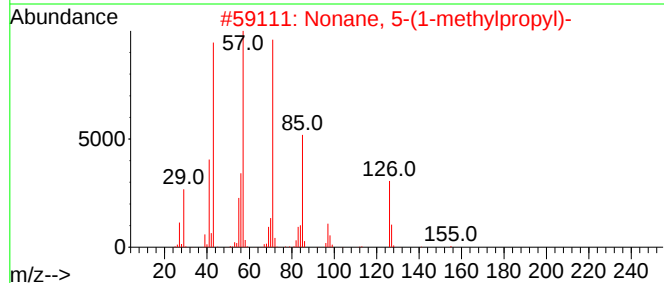
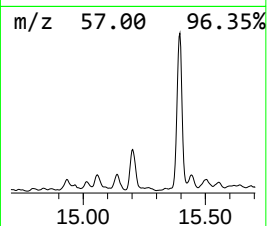
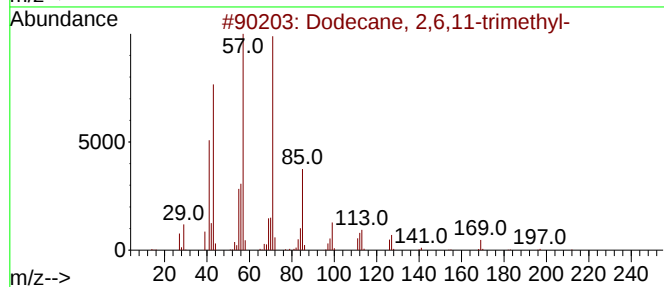
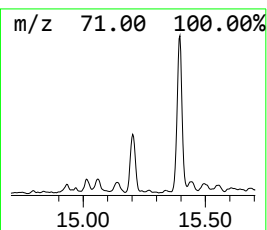
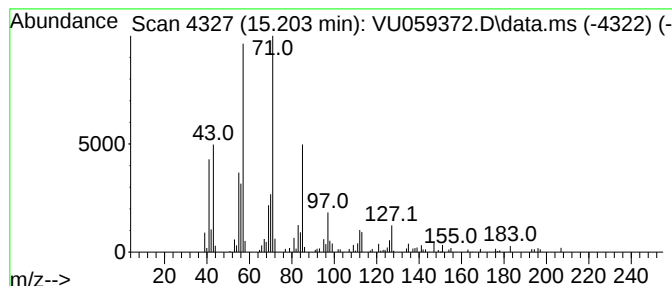
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Quant Title : VOC Analysis

TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

Peak Number 6 (DEL) Alkane: Straight-Chai... Concentration Rank 7

R.T.	EstConc	Area	Relative to ISTD	R.T.
15.203	7.32 ug/L	100132	1,4-Dichlorobenzene-d4	11.810

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Dodecane, 2,6,11-trimethyl-	212	C15H32	031295-56-4	78
2			Nonane, 5-(1-methylpropyl)-	184	C13H28	062185-54-0	64
3			Hexadecyl octyl ether	354	C24H50O	1000406-38-6	64
4			Undecane, 4,6-dimethyl-	184	C13H28	017312-82-2	59
5			Nonane, 5-butyl-	184	C13H28	017312-63-9	59



Data Path : Z:\voasrv\HPCHEM1\MSVOA_U\Data\VU062024\
Data File : VU059372.D
Acq On : 20 Jun 2024 12:10
Operator : MD/SY
Sample : P2897-07ME
Misc : 4.89g/5.0mL/100uL/5.0mL/MSVOA_U/MEOH
ALS Vial : 9 Sample Multiplier: 1

Instrument :
MSVOA_U
ClientSampleId :
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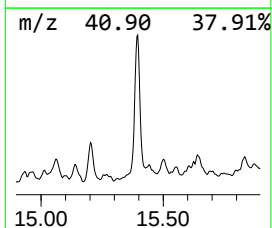
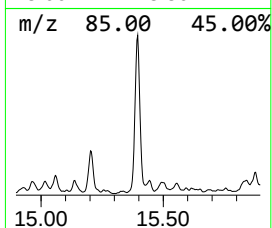
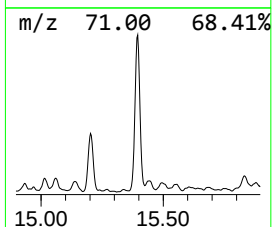
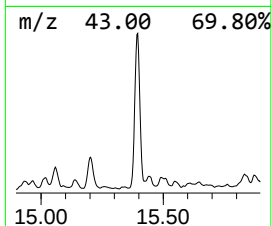
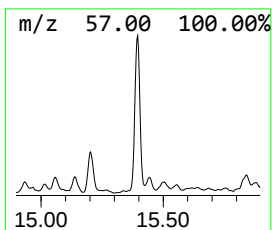
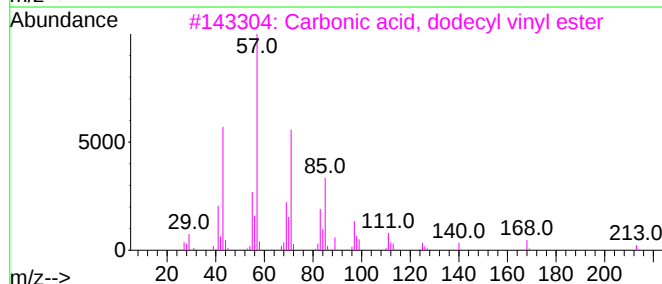
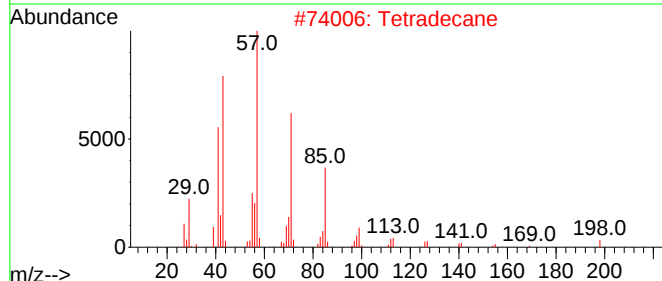
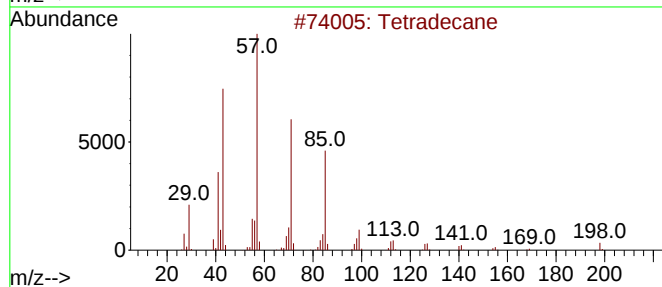
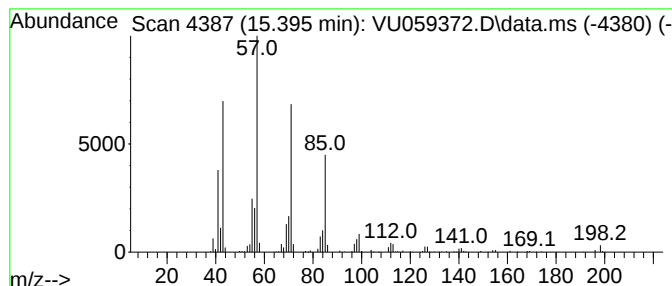
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Quant Title : VOC Analysis

TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

Peak Number 7 (DEL) Alkane: Straight-Chai... Concentration Rank 2

R.T.	EstConc	Area	Relative to ISTD	R.T.
15.396	19.55 ug/L	267330	1,4-Dichlorobenzene-d4	11.810

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Tetradecane	198	C14H30	000629-59-4	95
2			Tetradecane	198	C14H30	000629-59-4	94
3			Carbonic acid, dodecyl vinyl ester	256	C15H28O3	1000382-54-8	90
4			Tetradecane	198	C14H30	000629-59-4	90
5			Tridecane	184	C13H28	000629-50-5	90



Data Path : Z:\voasrv\HPCHEM1\MSVOA_U\Data\VU062024\
Data File : VU059372.D
Acq On : 20 Jun 2024 12:10
Operator : MD/SY
Sample : P2897-07ME
Misc : 4.89g/5.0mL/100uL/5.0mL/MSVOA_U/MEOH
ALS Vial : 9 Sample Multiplier: 1

Instrument :
MSVOA_U
ClientSampleId :
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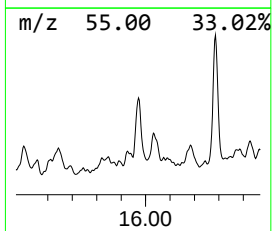
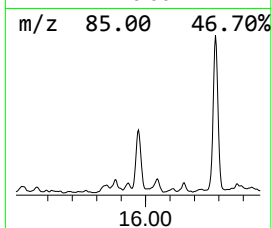
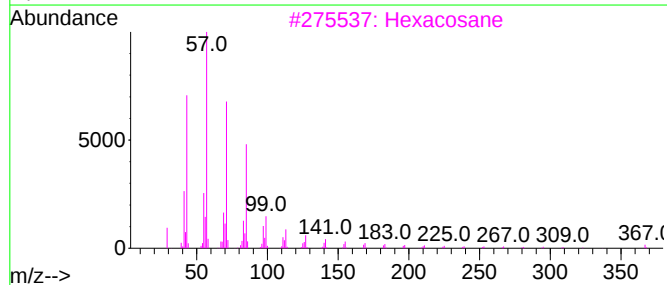
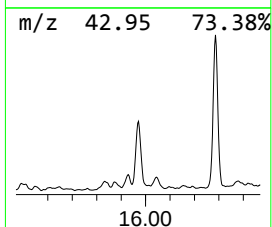
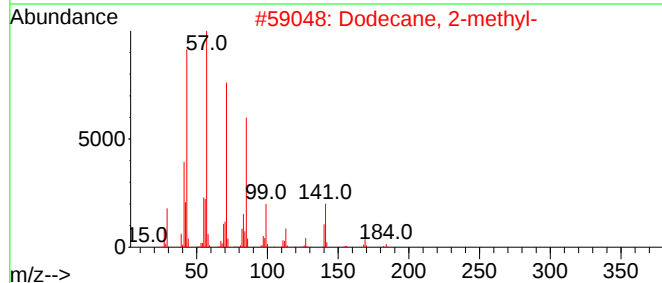
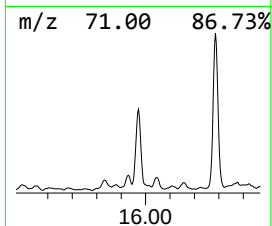
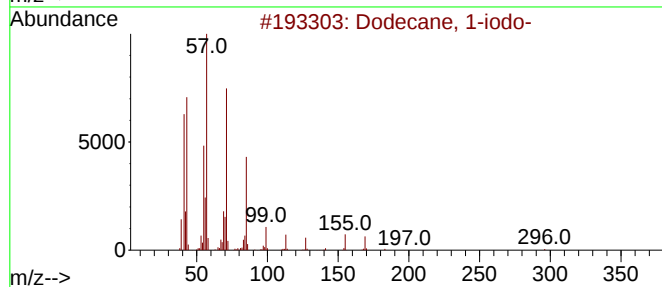
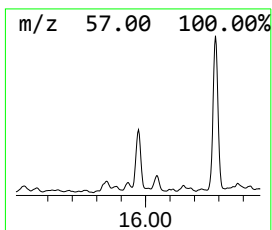
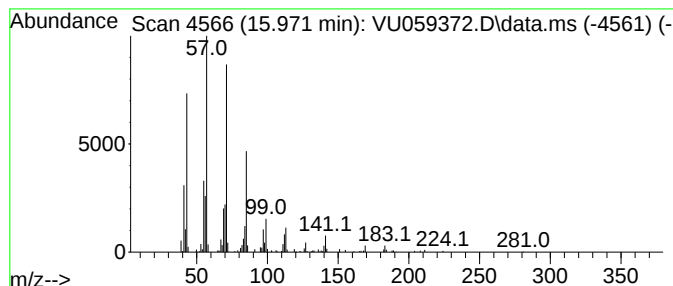
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Quant Title : VOC Analysis

TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

Peak Number 8 Dodecane, 1-iodo- Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.
15.971	14.12 ug/L	193100	1,4-Dichlorobenzene-d4	11.810

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Dodecane, 1-iodo-	296	C12H25I	004292-19-7	90
2			Dodecane, 2-methyl-	184	C13H28	001560-97-0	87
3			Hexacosane	366	C26H54	000630-01-3	86
4			Pentacosane	352	C25H52	000629-99-2	86
5			Heptadecane, 2,6,10,15-tetramethyl-	296	C21H44	054833-48-6	86



Data Path : Z:\voasrv\HPCHEM1\MSVOA_U\Data\VU062024\
Data File : VU059372.D
Acq On : 20 Jun 2024 12:10
Operator : MD/SY
Sample : P2897-07ME
Misc : 4.89g/5.0mL/100uL/5.0mL/MSVOA_U/MEOH
ALS Vial : 9 Sample Multiplier: 1

Instrument :
MSVOA_U
ClientSampleId :
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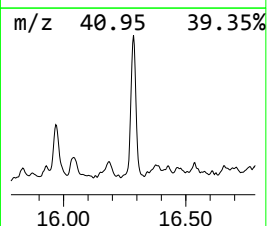
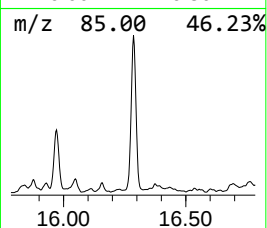
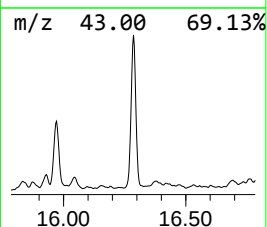
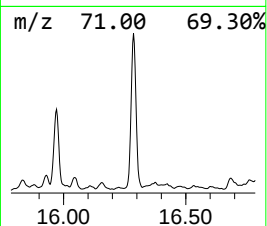
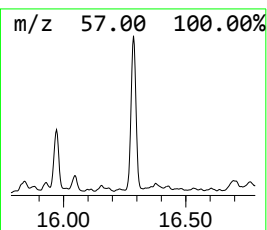
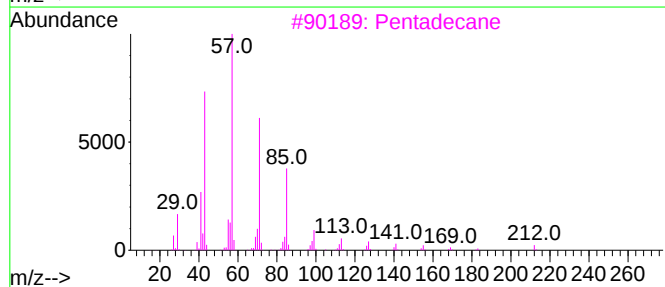
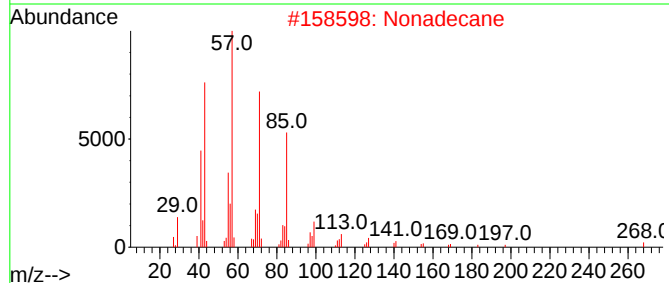
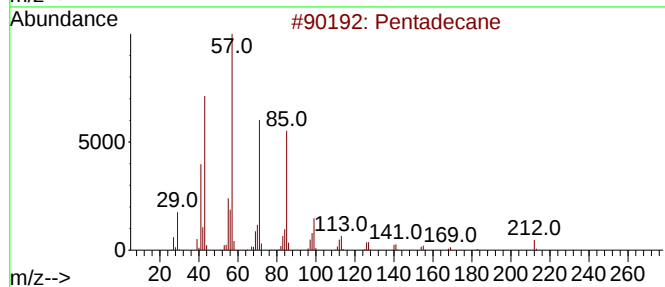
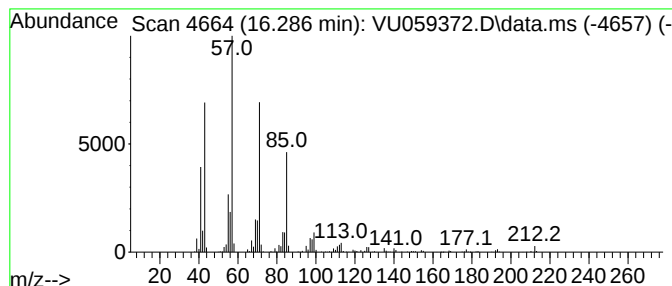
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Quant Title : VOC Analysis

TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

Peak Number 9 (DEL) Alkane: Straight-Chai... Concentration Rank 1

R.T.	EstConc	Area	Relative to ISTD	R.T.
16.286	33.49 ug/L	457849	1,4-Dichlorobenzene-d4	11.810

Hit#	of 5	Tentative ID	MW	MolForm	CAS#	Qual
1		Pentadecane	212	C15H32	000629-62-9	92
2		Nonadecane	268	C19H40	000629-92-5	91
3		Pentadecane	212	C15H32	000629-62-9	83
4		Tetradecane	198	C14H30	000629-59-4	80
5		Tetradecane	198	C14H30	000629-59-4	72



Data Path : Z:\voasrv\HPCHEM1\MSVOA_U\Data\VU062024\
Data File : VU059372.D
Acq On : 20 Jun 2024 12:10
Operator : MD/SY
Sample : P2897-07ME
Misc : 4.89g/5.0mL/100uL/5.0mL/MSVOA_U/MEOH
ALS Vial : 9 Sample Multiplier: 1

Instrument :
MSVOA_U
ClientSampleId :
C0SB7ME

Quant Method : Z:\voasrv\HPCHEM1\MSVOA_U\Method\SFAMULM052924WMA.M
Quant Title : VOC Analysis

TIC Library : C:\Database\NIST0.L
TIC Integration Parameters: LSCINT.P

TIC Top Hit name	RT	EstConc	Units	Response	--Internal Standard--			
					#	RT	Resp	Conc
Carbonic acid, ...	12.322	3.1	ug/L	41970	3	11.810	683617	50.0
Carbonic acid, ...	13.425	9.2	ug/L	125133	3	11.810	683617	50.0
(DEL) Alkane: S...	13.582	2.8	ug/L	37856	3	11.810	683617	50.0
(DEL) Alkane: S...	14.444	12.2	ug/L	166665	3	11.810	683617	50.0
(DEL) Alkane: S...	15.203	7.3	ug/L	100132	3	11.810	683617	50.0
(DEL) Alkane: S...	15.396	19.6	ug/L	267330	3	11.810	683617	50.0
Dodecane, 1-iodo-	15.971	14.1	ug/L	193100	3	11.810	683617	50.0
(DEL) Alkane: S...	16.286	33.5	ug/L	457849	3	11.810	683617	50.0